D-Glucitol 50-70-4 | DTXSID5023588

Model Performance

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Model	Data
110001	Bata

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 1.49 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.85e-01

Confidence level: 6.96e-01

Nearest Neighbors from the Training Set

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D-Glucitol

Measured: 1.45 Predicted: 1.49 Image not found

D-Mannitol Measured: 1.45 Predicted: 1.49

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D-Galactitol Measured: 1.45 Predicted: 1.49

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Xylitol

Measured: 4.22 Predicted: 2.97

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1-Propene-1,2,3-tricarboxylic

acid

Measured: 2.45 Predicted: 1.87

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1-Propene-1,2,3-tricarboxylic

Measured: 2.45 Predicted: 1.87

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d-Quercitol

Measured: 6.70e-01 Predicted: 6.94e-01

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Shikimic acid

Measured: 8.61e-01 Predicted: 9.67e-01